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Few-body problems involving Coulomb or gravitational interactions between pairs of particles, whether in classical or quantum physics, are generally handled through a standard multipole expansion of the two-body potentials. We discuss an alternative based on a compact, cylindrical Green's function expansion that should have wide applicability throughout physics. Two-electron "direct" and "exchange" integrals in many-electron quantum systems are evaluated to illustrate the procedure which is more compact than the standard one using Wigner coefficients and Slater integrals.

I. INTRODUCTION

For pairwise Coulomb or gravitational potentials, one often expands the inverse distance between two points $\mathbf{x}$ and $\mathbf{x}'$ in the standard multipole form [1]

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|} = \frac{1}{\sqrt{rr'}} \sum_{\ell=0}^{\infty} \left(\frac{r_<}{r_>}\right)^{\ell+\frac{1}{2}} P_\ell(\cos\gamma), \tag{1}$$

where $r_<$ ($r_>$) is the smaller (larger) of the spherical distances r and r', and $P_\ell(\cos\gamma)$ is the Legendre polynomial [2] with argument

$$\cos\gamma \equiv \hat{\mathbf{x}}\cdot\hat{\mathbf{x}}' = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\phi-\phi'). \tag{2}$$

In the "body frame," separation distances within the set composed of two points and the origin are characterized by three variables, one choice being the above triad ($r_<$, $r_>$, γ). With respect to a space-fixed "laboratory frame," three more angles constitute the full set of six coordinates, the choice in Eq. (2) of (θ, θ', $\phi-\phi'$) being suited to the spherical polar coordinates of the individual vectors; thus, $\mathbf{x}$: ($r\sin\theta\cos\phi$, $r\sin\theta\sin\phi$, $r\cos\theta$).

The multipole expansion in spherical polar coordinates is almost universal because we treat particles or charges as points. Thus, in the three-body problem, once the motion of the center of mass is separated, we are left with two vectors which may be described as in the above paragraph, the potential energy and thereby dynamics in the body frame being a function of the three dynamical variables ($r_<$, $r_>$, γ). In this paper, we present an alternative expansion to Eq. (1) based on cylindrical (azimuthal) symmetry which may be of wide interest in physics and astrophysics. As an illustration, we evaluate two-electron integrals expressing the "direct" and "exchange" components of the electron-electron repulsion in atoms.

The expansion in Eq. (1) disentangles the dynamics contained in the radial variables from symmetries, particularly under rotations and reflections, pertaining to the angle γ. Whereas the three variables at this stage are joint coordinates of $\mathbf{x}$ and $\mathbf{x}'$, depending on both and thus characteristic of the three-body system as a whole, a further disentangling in terms of the independent coordinates so as to handle permutational and rotational symmetry aspects of the problem is often useful and achieved through the addition theorem for spherical harmonics [3]. Using this to replace $P_\ell(\cos\gamma)$ in Eq. (1), we obtain the familiar Green's function multipole expansion in terms of all six spherical polar coordinate variables $\mathbf{x}$ and $\mathbf{x}'$,

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|} = \frac{1}{\sqrt{rr'}} \sum_{\ell=0}^{\infty} \left(\frac{r_<}{r_>}\right)^{\ell+\frac{1}{2}} \sum_{m=-\ell}^{\ell} \frac{\Gamma(\ell-m+1)}{\Gamma(\ell+m+1)} P_\ell^m(\cos\theta) P_\ell^m(\cos\theta') e^{im(\phi-\phi')}, \tag{3}$$

where $P_\ell^m(z)$ is the integer-order, integer-degree, associated Legendre function of the first kind [2]. Apart from the first factor with dimension inverse-distance formed from the geometric mean of the two lengths r and r', this expression involves only four combinations: $(r_</r_>, \theta, \theta', \phi - \phi')$ of the six coordinates $\mathbf{x}$ and $\mathbf{x}'$. This is as it should be, the separation distance being independent of the orientation of that separation in the laboratory frame, and thus independent of two angles serving to specify that orientation.

This multipole expansion is very broadly utilized across the physical sciences. With ℓ and m interpreted as the quantum numbers of orbital angular momentum and its azimuthal projection, respectively, a whole technology of Racah-Wigner or Clebsch-Gordan algebra is available [4] for handling all angular (that is, geometrical or symmetry) aspects of an N-body problem, the dynamics being confined to radial matrix elements of the coefficients $(r_</r_>)^{\ell+1/2}$ in Eq. (1). Although many other systems of coordinates have been studied for problems with an underlying symmetry that is different from the spherical, Eq. (1), in combination with the addition theorem for spherical harmonics, has gained such prominence as to have become the Green's function expansion of choice even for non spherically-symmetric situations.

II. ALTERNATIVE FOURIER EXPANSION

In a recent investigation [5] of gravitational potentials in circular cylindrical coordinates $\mathbf{x}$: (R, ϕ, z), two of us discovered and used an expansion

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|} = \frac{1}{\pi\sqrt{RR'}} \sum_{m=-\infty}^{\infty} Q_{m-\frac{1}{2}}(\chi)\; e^{im(\phi-\phi')}, \tag{4}$$

with $Q_{m-\frac{1}{2}}$ a Legendre function of the second kind of half-integer degree [6], and χ defined as

$$\chi \equiv \frac{R^2 + {R'}^2 + (z-z')^2}{2RR'} = \frac{r^2 + {r'}^2 - 2rr'\cos\theta\cos\theta'}{2rr'\sin\theta\sin\theta'}. \tag{5}$$

We have since uncovered this expansion as an application of the "Heine identity" in the literature [7, 8],

$$\frac{1}{\sqrt{v-\cos\psi}} = \frac{\sqrt{2}}{\pi} \sum_{m=-\infty}^{\infty} Q_{m-\frac{1}{2}}(v)\; e^{im\psi}, \tag{6}$$

which has a long history but seems not to have been exploited in mathematical physics in recent times. However, we have found it powerful for problems with a cylindrical geometry and have used it for compact numerical evaluation of gravitational potential fields of several axisymmetric and nonaxisymmetric mass distributions [5]. We now set Eq. (4) in a broader context, together with new associated addition theorems and an application in quantum physics, hoping to encourage wider use of this expansion throughout physics.

The expansion in Eq. (4), may be viewed either, in analogy with Eq. (1), as an expansion in Legendre functions, now of the second kind in the joint variable χ of the whole system, with coefficients $(RR')^{-1/2}e^{im(\phi-\phi')}$, or as a Fourier expansion in the variable $(\phi - \phi')$ with the Q's as coefficients. In this latter view, a further step allows us to develop a new addition theorem for these Legendre functions. Interchanging the ℓ and m summations in Eq. (3), we obtain

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|} = \frac{1}{\sqrt{rr'}} \sum_{m=-\infty}^{\infty} e^{im(\phi-\phi')} \sum_{\ell=|m|}^{\infty} \left(\frac{r_<}{r_>}\right)^{\ell+\frac{1}{2}} \frac{\Gamma(\ell-m+1)}{\Gamma(\ell+m+1)} P_\ell^m(\cos\theta) P_\ell^m(\cos\theta'). \tag{7}$$

Comparing with Eq. (4), we obtain a new addition theorem, this time for the Legendre function of the second kind,

$$Q_{m-\frac{1}{2}}(\chi) = \pi\sqrt{\sin\theta\sin\theta'} \sum_{\ell=|m|}^{\infty} \left(\frac{r_<}{r_>}\right)^{\ell+\frac{1}{2}} \frac{\Gamma(\ell-m+1)}{\Gamma(\ell+m+1)} P_\ell^m(\cos\theta) P_\ell^m(\cos\theta'). \tag{8}$$

Note that $Q_{m-\frac{1}{2}} = Q_{-m-\frac{1}{2}}$ as per Eq.(8.2.2) in [2].

Similarities and contrasts between the pairs of equations, Eqs. (1) and (3) and Eqs. (4) and (8), are worth emphasizing. Of the four variables $(r_</r_>, \theta, \theta', \phi - \phi')$, the first pair of equations expresses the inverse distance as a series in powers of the first variable with coefficients Legendre polynomials of the first kind in γ, a composite of the other three variables and decomposable in terms of them through the addition theorem as in Eq. (3). The second pair of equations, on the other hand, expands in Eq. (4) the inverse distance in terms of the variable $\phi - \phi'$, with expansion coefficients Legendre functions of the second kind in χ, a composite of the other three variables $(r_</r_>, \theta, \theta')$ and decomposable in terms of them through the addition theorem in Eq. (8). For this comparison, it is useful to recast Eq. (1) in the more suggestive form,

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|} = \frac{1}{\sqrt{rr'}} \sum_{\ell=0}^{\infty} P_\ell(\cos\gamma)\; e^{-(\ell+\frac{1}{2})(\ln r_> - \ln r_<)}. \tag{9}$$

Whereas this expansion has half-integers in the exponents and integer degree Legendre polynomials of the first kind, Eq. (4) has integer m's in the exponents and half-integer degree Legendre functions of the second kind.

Yet another alternative to Eq. (4) follows upon casting the square root in the expression for the distance in terms of r, r', and γ in the form Eq. (6) through the definition

$$v \equiv \frac{1}{2}\left(\frac{r_<}{r_>} + \frac{r_>}{r_<}\right) = \frac{r^2 + r'^2}{2rr'}. \tag{10}$$

This gives the expression

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|} = \frac{1}{\pi\sqrt{rr'}} \sum_{n=-\infty}^{\infty} Q_{n-\frac{1}{2}}(v)\; e^{in\gamma}, \tag{11}$$

now a Fourier expansion in γ instead of the $(\phi - \phi')$ of Eq. (4), with $Q_{n-\frac{1}{2}}(v)$ as the coefficients. In terms of hyperspherical coordinates, widely used in atomic and nuclear study of three (or more) bodies [9], the variable v is $\csc 2\alpha$, α being a "hyperangle".

We present in this paragraph a number of alternative expressions for the functions $Q_{m-\frac{1}{2}}$ which are useful in calculations using such expansions as Eqs. (4) and (11). Setting $\theta = \theta' = \pi/2$ in Eq. (8) and using Eq. (8.756.1) of [10] gives

$$Q_{m-\frac{1}{2}}(v) = \pi \sum_{\ell=|m|}^{\infty} \left(\frac{r_<}{r_>}\right)^{\ell+\frac{1}{2}} \frac{\Gamma(\ell-m+1)}{\Gamma(\ell+m+1)} \frac{\pi 2^{2m}}{[\Gamma(1+\frac{\ell-m}{2})\Gamma(\frac{1-\ell-m}{2})]^2}, \tag{12}$$

which can be rewritten as

$$Q_{m-\frac{1}{2}}(v) = \pi e^{-(m+\frac{1}{2})\eta} \sum_{\ell=0}^{\infty} 2^{1-2m-4\ell} \binom{2\ell}{\ell} \binom{2\ell+2m-1}{\ell+m} e^{-2\ell\eta}, \tag{13}$$

where we have defined $r_</r_> \equiv e^{-\eta}$, $v = \cosh\eta$. Although the ℓ-th term of these series is in different form from what one obtains through the more familiar formula for Q as a hypergeometric function [11], namely,

$$Q_{m-\frac{1}{2}}(v = \cosh\eta) = \frac{\sqrt{\pi}\,\Gamma(m+\frac{1}{2})}{\Gamma(m+1)} e^{-(m+\frac{1}{2})\eta}\; {}_2F_1(\frac{1}{2}, m+\frac{1}{2}; m+1; e^{-2\eta}), \tag{14}$$

their equivalence follows from straightforward algebra. Also, another standard expansion for Q in powers of v as in Eq. (8.1.3) of [2],

$$Q_{\nu-\frac{1}{2}}(v) = \frac{\sqrt{\pi}\,\Gamma(\nu+\frac{1}{2})}{\Gamma(\nu+1)} (2v)^{-\nu-\frac{1}{2}}\; {}_2F_1(\frac{\nu}{2}+\frac{3}{4}, \frac{\nu}{2}+\frac{1}{4}; \nu+1; \frac{1}{v^2}), \tag{15}$$

is equivalent. However, the results directly in powers of $r_</r_>$ in Eqs. (12) , (13), and (14) are more convenient in many applications. Among specific features worth noting in these alternative expansions are that only even powers of $(r_</r_>)$ occur in the sum in Eq. (13) and that for any m, the sum in Eq. (12) runs over all ℓ values compatible with it, $\ell \geq |m|$, as per their interpretation as angular momentum quantum numbers.

In the multipole expansion in Eq. (1), γ is an angle formed out of the set $(\theta, \theta', \phi - \phi')$ and, therefore, $\cos\gamma$ in the functions P_ℓ has range of variation from -1 to 1. On the other hand, in the expansions in Eqs. (4) and (6), the arguments v and χ of the Legendre functions of the second kind range from 1 to infinity and, therefore, can be written in terms of hyperbolic functions as $\cosh\eta$ and $\cosh\xi$, respectively. From Eq. (5) we have the link between them,

$$\cosh\eta = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cosh\xi. \tag{16}$$

This disentanglement of v (or η) in terms of a triad is the counterpart of Eq. (2) and may be used with addition theorems given in the literature such as [7, 8]

$$Q_{m-\frac{1}{2}}(\cosh\eta) = \sum_{n=-\infty}^{\infty} (-1)^n \frac{\Gamma(m-n-\frac{1}{2})}{\Gamma(n+m-\frac{1}{2})} Q^n_{m-\frac{1}{2}}(\cos\theta) P^n_{m-\frac{1}{2}}(\cos\theta')\ e^{n\xi}. \tag{17}$$

III. TWO-ELECTRON INTEGRALS

We contrast usage of the alternative expansions in Eqs. (1) and (4) for calculating the electrostatic interaction as it appears in atomic, molecular and condensed matter physics. Thus, consider the so-called "direct" part of this interaction between two electrons in the $3d^2$ configuration,

$$V^D_{ee} = \int\int d\mathbf{x}d\mathbf{x}' \psi^*_{3d}(\mathbf{x})\psi^*_{3d}(\mathbf{x}')|\mathbf{x}-\mathbf{x}'|^{-1}\psi_{3d}(\mathbf{x})\psi_{3d}(\mathbf{x}'). \tag{18}$$

The standard treatment [12] uses Eqs. (1) and (3), carries out all the angular integrals through Racah-Wigner algebra, leaving behind radial "Slater integrals" $F^k(dd), k = 0, 2, 4$, and yielding (for illustrative purposes, all m values have been set equal to zero)

$$V^D_{ee} = F^0(dd) + (4/49)F^2(dd) + (36/441)F^4(dd), \tag{19}$$

where the coefficients are evaluated in terms of Wigner $3j$-symbols or are available in tables [12]. The Slater integrals,

$$F^k(dd) = \int\int r^2 dr r'^2 dr' (r^k_</r^{k+1}_>) R^2_{3d}(r) R^2_{3d}(r'), \tag{20}$$

remain for numerical evaluation. In this example, upon evaluation with hydrogenic radial functions, we obtain $V = 0.092172$ in atomic units. The alternative calculation through Eq. (4) involves only the $m = 0$ term and thereby the integral

$$V^D_{ee} = \frac{1}{\pi}\int\int\int\int R^{1/2}dR R'^{1/2}dR' dz dz' Q_{-\frac{1}{2}}(\chi)|\psi_{3d}(\mathbf{x})|^2|\psi_{3d}(\mathbf{x}')|^2. \tag{21}$$

The integrand is a function of z and R variables alone and our numerical evaluation of this integral reproduces the value cited above.

As a second example, we computed an exchange integral for the $3d4f$ configuration again setting, for simplicity, all m equal to zero:

$$V^E_{ee} = \int\int d\mathbf{x}d\mathbf{x}' \psi^*_{3d}(\mathbf{x})\psi^*_{4f}(\mathbf{x}')|\mathbf{x}-\mathbf{x}'|^{-1}\psi_{3d}(\mathbf{x}')\psi_{4f}(\mathbf{x}). \tag{22}$$

The standard method through exchange Slater integrals G and Wigner coefficients gives [12]

$$V^E_{ee} = (9/35)G^1(df) + (16/315)G^3(df) + (500/7623)G^5(df) \tag{23}$$

and, again through hydrogenic radial functions, gives the value $V^E_{ee} = 0.0082862$. We reproduce the same result upon directly computing Eq. (22) with Eq. (4), again involving a single four-dimensional integral as in Eq. (21) with $Q_{-\frac{1}{2}}$.

As the orbital angular momenta involved of the two electrons increase, the number of terms in expressions such as Eqs. (19) and (23) also grows, necessitating the computing of more Wigner coefficients and Slater integrals. By contrast, only a single term of the expansion in Eq. (4) and a single integral is necessary in our suggested alternative, the ϕ integrations setting $m = 0$ for direct terms and m equal to the difference in the m values of the two orbitals for exchange terms. Of course, the price paid is that four-dimensional integrations are needed unlike the two-dimensional ones in the Slater integrals. This same selection rule imposed by the ϕ integrations means that even in a calculation with several configurations and the imposition of antisymmetrization, such as in a multi-configuration Hartree-Fock scheme, matrix elements of $|\mathbf{x}-\mathbf{x}'|^{-1}$ between each term in the bra and in the ket gets a contribution from only one m value in the expansion in Eq. (4).

IV. SUMMARY

The inverse distance between two points $\mathbf{x}'$ and $\mathbf{x}$ is intimately involved in Coulomb and gravitational problems. Its expansion in terms of Legendre polynomials P_ℓ of the angle between the vector pair or a further double-summation expansion involving the individual polar angles of the vectors are well known and widely used in physics and astronomy. We have discussed an alternative in terms of cylindrical coordinates, a single summation in terms of Legendre functions $Q_{m-\frac{1}{2}}$ of the second kind in a pair variable χ or double summations involving the individual coordinates. These expansions are better suited to problems involving cylindrical (azimuthal) symmetry as shown by applications in [5] and by an illustration here for very common electron-electron calculations throughout many-electron physics. Further variants are possible for other coordinates such as ring or toroidal, parabolic, bispherical, cyclidic and spheroidal [13], and we plan to return to them in future publications. Connections to the theory of Lie groups will also be of interest [14].

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